**CHEMICAL ENGINEERING TRANSACTIONS**, Volume 7, 2005
Edited by Jiří Klemeš


# On pollution minimization in the optimization models of process network synthesis

C. Imreh and Z. Kovács
Department of Informatics, University of Szeged
Árpád tér 2, H-6720 Szeged, Hungary
E-mail: cimreh@inf.u-szeged.hu and kovacsz@inf.u-szeged.hu

Novel mathematical models are developed for taking into account the pollution of processes in Process Network Synthesis (PNS). Initially the combinatorial mathematical model of PNS is extended to handle the pollutions of processes. The resultant model is called PCPNS (Pollution Constrained PNS). An algorithm is elaborated for solving this optimization problem. Finally a second mathematical model is introduced for defining PNS problems quantitatively.

## 1. Introduction

In a manufacturing system physical and/or chemical states of material are changed through various physical and/or chemical transformations to yield desired products. Functional units performing these transformations are called operating units. A manufacturing system can be considered as a network of operating units which is called process network. The need for minimizing the cost of process networks is obvious.

On the other hand nowadays the cost minimization is not the only goal which must be considered. From environment protection point of view it is also an important goal to design systems resulting in minimal possible pollution. In many cases several laws and regulations force the industry to take the pollution into account in the design of process networks. In the present work mathematical models are developed to take into account pollution of the processes. First a combinatorial model is introduced where a pollution value is assign to each transformation. These values supposed to be constant parameters of the operating units modeling the transformations. A more general quantitative model is also presented where pollution functions are assigned to the materials to define the pollution of the system.

The paper is organized as follows. In the next section the combinatorial mathematical model of PNS problem is extended to a more general one capable of handling the problem described. In Section 3 the pollution constrained model is detailed and an algorithm is presented for solving the model. Furthermore, it is sketched how to modify the algorithm to handle different models. In Section 4 the quantitative model is considered as a generalization of the quantitative model of the PNS. The paper is closed

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This research was partially supported by the Hungarian Science Foundation Grant No. OTKA T046405

by Section 5 summarizing the main results and listing the most important open questions related to the models developed in this paper.

## 2. Combinatorial mathematical model

Let $M$ be a finite nonempty set, the set of the materials. The candidate transformations are presented as operating units, each of which is given by two sets of materials, i.e., the set of input materials to and the set of output materials from the operating unit. The set of all operating units is denoted by $O$. The process graph or P-graph in short is defined by pair $(M, O)$. The set of vertices of this directed graph is $M \cup O$, and the set of arcs contains *i)* the edges leading to an operating unit from its input materials and *ii)* the edges leading from an operating unit to its output materials. Then some subgraphs of the P--graph describes feasible processes which are able to produce the required materials from the raw materials. Friedler at al. (1992) show that a subgraph $(m,o)$ belongs to a feasible process if and only if it satisfies the following properties.
*(A1)* P is a subset of $m$.
*(A2)* a material from $m$ is a raw material if and only if no edge goes into it in the P-graph $(m, o)$.
*(A3)* for every operating unit of $o$ there exists a path in the P-graph $(m,o)$ which goes from $o$ into a desired product.
*(A4)* all of the materials in $m$ are either input or output material of some operating unit from set $o$.
The subgraphs which satisfy the above properties are called feasible solutions. The set of the feasible solutions is denoted by $S(M)$. This combinatorial approach of the processes is detailed in article Friedler et al. (1992).

In the combinatorial model each operating unit has a cost (a nonnegative value), which gives the cost of the transformation modeled by the operating unit. The goal is to find such feasible solution where the total cost of the used operating units (contained in set o) is minimal. This is a combinatorial optimization problem. Blázsik and Imreh (1996) proved that the problem belongs to the class of NP-complete problems. This is the complexity class of the hard optimization problems in other words it is not expected to find effective, polynomial time algorithms to solve the problem. Some exponential time algorithms were developed for the solution of the problem (see Imreh and Magyar, 1998), and heuristic algorithms were also developed (Blázsik et al. 1999), moreover some special problem classes that can be solved in polynomial time were also investigated (Imreh 2001).

If we extend the combinatorial model to handle the pollution belonging to the possible transformation of the processes also, we can still use the P-graph representation. However in our case the operating units (the possible transformations) have an additional parameter which describes the environment pollution belonging to the operating unit. In the combinatorial model this parameter is presented by a pollution value which is a nonnegative number.

In this generalized model different questions arise. One question is if a bound - which is called pollution bound and denoted by PB - is given on the maximal total amount of the possible pollution of the overall process how to find the cheapest process which does not violate this bound on the possible pollution. We call this model the pollution constrained PNS model (PCPNS in short). In the mathematical model this means that among the feasible solution whose total pollution value is not more than PB - we call these feasible solution PC-feasible solutions - we have to find the P-graph where the total cost is minimal. A similar question is if we have a bound on the total cost how to find the process which has the smallest total pollution value, this model is called cost constrained PNS problem and denoted by CCPNS in short. Another model is where a mixed objective function is to be minimized, which is usually monotone and convex function of the total cost and the total pollution value. This model is called the mixed objective PNS model (MOPNS in short).

## 3. Algorithm for the PCPNS problem

In this section we present an algorithm based on the branch-and-bound technique which solves the PCPNS optimization problem. In the algorithm we use the concept of the decision mapping which was introduced by Friedler et al (1995). For an arbitrary material $m$ denote by $\Delta(m)$ the set of operating units which produce the material. Then we can define a mapping $\delta$ on the set of materials which assigns to each material $m$ a set $\delta(m)$ which is a subset of $\Delta(m)$. The decision mapping defines for the material which operating units produce it in the process network considered. On the other hand some decision mappings are contradictory. For example, if such operating units whose output set contains a material X are selected to produce in a solution a material Y, then they must be also selected to produce X as well. To avoid this contradiction the consistent decision mappings are defined. A decision mapping is called consistent if for an arbitrary pair of materials X, Y it is valid that $\delta(X) \cap \Delta(Y)$ is a subset of $\delta(Y)$. Then for each feasible solution of the combinatorial PNS problem we can give a consistent decision mapping which describes for each material the set of the selected operating units producing it. Using the decision mapping we can build an algorithm for the solution of the PCPNS problem.

The algorithm is based on the branch and bound technique (see Beale 1979 for detailed description). The technique can be used to solve combinatorial optimization problems where we are to find the minimum of a function $z$ a finite discrete set $L$ of the feasible solutions. The technique based on the following two functions. One of the functions is the branching function $\Psi$. In the basic procedure it assigns a real partition to an arbitrary at least two-elements set of the feasible solutions. In a more advanced version we consider a larger set which contains the set of feasible solutions, and the branching function is defined on this larger set. The other function is $g$ which gives a lower bound on the possible values of the objective function in the set of feasible solutions considered. It is required that in the case where the set contains only one feasible solution then $g$ gives the objective function value for the set. If we can define such functions then the branch and bound technique solves the problem as follows.

Branch and Bound procedure:
*Initialization:* Let the root of the tree $L$ and calculate $g(L)$ as the label of root. Let r=1.
*Iteration Part* (*r-th iteration*):
*Step 1.* Choose among the levels of the tree a point which has the minimal label. Denote this set of feasible solutions by $L'$.
*Step 2.* If $L'$ contains only one feasible solution, then the procedure is finished this element is the optimal solution.
*Step 3.* Consider the sets received by $\Psi(L')$, delete the sets which do not contain feasible solutions and determine the function $g$ for each remaining set. Assign this value as a label to them and extend the tree with these sets, they become the children of $L'$. Increase $r$ by 1, and go to the next iteration.

Now let us examine, how can we use this framework for the solution of the PCPNS problem. We can use the decision mapping to define the branching function. The sets which are contained in the tree will be characterized by two parameters, some materials called fixed materials will be given with their decision mapping value and in the meantime some other materials called desired materials will be given. Such feasible solutions are contained in the set where these materials are produced and the fixed materials are produced by the operating units described by the decision mapping. At the beginning in the root $L$ contains all of the feasible solutions this set is characterized by the required products. The branching function chooses one material and divides the set of feasible solutions by considering all of the decision mapping values for the material which are consistent with the earlier decisions. For each decision mapping value the new set of feasible solutions is characterized as follows. The set of the fixed materials is extended with the considered material and the value of the decision mapping. Furthermore in the new set the input materials of the operating units selected by the decision mapping which are not contained in the fixed or desired set are placed into the set of desired materials.

Now let us consider the bounding function. The simplest bound which can be used is the total cost of the operating units selected by the decision mapping values of the fixed materials. We can use a better bound if we determine the path in the P-graph which has the smallest cost (the cost of a path is the total cost of its operating units) among the paths connecting a raw material with a desired or a fixed material. We can increase the bound received by the decision mapping with the cost of that path. Other more complicated bounding functions are given by Imreh and Magyar (1998).

Finally let us consider the role of the pollution constraint. This constraint can be used in Step 3. to eliminate some sets which do not contain feasible solution of the PCPNS problem. In the case where the total pollution of the operating units selected by the decision mapping for the fixed materials is more then the pollution constraint, then the set cannot contain feasible solutions. For a set let us determine the path in the P-graph which has the smallest pollution value (the pollution value of a path is the total pollution value of the operating units in it) among the paths connecting a raw material with a desired or a fixed material. If the sum of the pollution value of the selected operating units and the pollution value of that path violate the pollution constraint, then we can also eliminate this set in Step 3.

Concerning the other combinatorial models defined in the previous section, we can build similar procedures. Since in our model the role of the cost and the pollution value is symmetric the above presented procedure can be easily modified to solve the CCPNS model. The same structure can be used to solve the MOPNS problem. However, in this case we cannot use the pollution constraint to exclude sets in Step 3. Furthermore we have to define other bounding functions depending on the function used in the model.

## 4. Extension to the quantitative model

In this section we examine the quantitative PNS model, which is a more complex model than the combinatorial one, and leads to a nonlinear optimization problem. This model was introduced by Friedler at al. (1998).

In this model it is supposed that the cost of an operating unit not a constant it depends on the materials used and produced by it. We describe a process network by the following variables. We assign a decision variable $y_i$ to each operating unit which takes value 1, if the operating unit is selected in the solution, value 0, if it is not. For each edge $a_j$ in the P-graph we define a variable $x_j$, which gives the quantity of the materials belonging to the edge (the input material, if the edge goes into an operating unit, the output material if the edge goes from an operating unit). For an arbitrary set $E$ of edges denote by $\varphi(E)$ the set of the corresponding x variables. Furthermore for an arbitrary operating unit $o_j$ let us denote by $in(o_j)$ the set of the incoming edges and by $out(o_j)$ the set of outgoing edges. For each operating unit we have some rules about the quantities of the incoming and outgoing materials, in most cases this rule can be described as a bound on a function (usually nonlinear) of the quantities. This means that in the mathematical model, for each operating unit $o_j$ there is a function $g_j$ and the bound on the quantities can be written in the form $g_j\,(\varphi(in(o_j)),\ \varphi(out(o_j)),y_j) \leq 0$. The cost of an operating unit can also depend on the materials used and produce by it, this cost is given by a function $f_j$, and the cost of the operating unit is $f_j\,(\varphi(in(o_j)),\ \varphi(out(o_j)),y_j)$.

Concerning the materials we can denote by $in(m_j)$ the set of the incoming edges into material $m_j$ and by $out(m_j)$ the set of outgoing edges from material $m_j$. Then the bound on the materials we must produce everything which is used can be described by a bound on some usually linear function $g'_j$ as $g'_j\,(\varphi(in(m_j)),\ \varphi(out(m_j))) \leq 0$. It is worth noting that in a more general model a cost is assigned to the materials which is also a function of $\varphi(in(m_j))$ and $\varphi(out(m_j))$. If we consider the optimization problem where the objective is to minimize $\sum f_j$ and the constraints are given by the $g_j$ and $g'_j$ functions furthermore we require that the selected ($y_j$=1) operating units satisfy the properties A1, A2, A3, A4, then we obtain a quantitative model of the PNS problem which is a nonlinear optimization problem.

Now let us investigate how can we modify the model to consider pollution. For each operating unit we can define a pollution value which may depend on the quantities of the input and produced materials, this can be given by a function $p_j$, and the pollution value of the operating unit is $p_j\ (\varphi(in(o_j\ )),\ \varphi(out(o_j\ )),\ y_j)$. Moreover we can assign independently a pollution value to the materials which may depend on the produced and the used amount, thus we can describe it by a function $p'_j$ as $p'_j\ (\varphi(in(m_j\ )),\ \varphi(out(m_j\ )))$. In this case the total pollution value of the process network is $\sum p_j + \sum p'_j$. After the definition of the pollution value of a process network we can define the models PCPNS, CCPNS, MOPNS in the same way as in the combinatorial case.

## 5. Summary and further questions

A novel mathematical model has been presented which makes it possible to take into account the environment pollution of the processes during the synthesis of process networks. A precise mathematical description of this model has been introduces extending the combinatorial PNS model based on the P-graph representation. An algorithm has been elaborated for solving the optimization problem resulted from pollution constrained model of PNS. An extension of the model has been given for a more general quantitative PNS model.

There are many further questions to be solved. Concerning the combinatorial models it is an interesting question to develop more sophisticated branch and bound algorithm by using more refined bounding functions and test these procedures. Since the problem is NP-hard from the complexity theory point of view it is an interesting problem to develop and analyze heuristic algorithms for the solution of the problem.

## 6. References

Beale, E. M. L., 1970, Branch and Bound Methods for mathematical programming system, Annals of Discrete Mathematics, vol. 5, 201—219.

Blázsik Z., Imreh B., 1996, A Note on Connection between PNS and Set Covering Problems, Acta Cybernetica, vol. 12, 309—312.

Blázsik Z., Holló Cs., Imreh Cs., Kovács Z., 1999, Heuristics for the PNS problem, Optimization Theory, Mátraháza, Applied Optimization, vol. 59, Eds. F. Gianessi, P. Pardalos, T. Rapcsák, Kluwer Academic Publishers, Dordrecht, Boston, London, 2001, 1—18.

Friedler F., Fan L. T., Imreh, B., 1998, Process Network Synthesis: Problem Definition, Networks, vol. 28, 119--124.

Friedler F., Tarján K., Huang Y. W., and Fan L. T., 1992, Graph-Theoretic Approach to Process Synthesis: Axioms and Theorems, Chem. Eng. Sci., vol. 47(8), 1973—1988.

Friedler F, J. B. Varga, L. T. Fan, 1995, Decision mappings: a tool for consistent and complete decisions in process synthesis, Chem. Eng. Sci, vol.. 50(11), 1755—1768.

Imreh, B., G. Magyar, 1998, Empirical Analysis of Some Procedures for Solving Process Network Synthesis Problem, Journal of Computing and Information Technology, vol. 6, 372—382.

Imreh Cs., 2001, New well-solvable class of PNS problems, Computing, vol. 66, 289—296.